

Thiamine disulfide

67-16-3 | DTXSID6046890

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.75×10^{-10} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 5.02×10^{-2}

Confidence level: 8.19×10^{-1}

Nearest Neighbors from the Training Set

Image not found

alpha-Humulene

Measured: 2.90×10^{-10}

Predicted: 2.87×10^{-10}

Image not found

Myrcene

Measured: 2.15×10^{-10}

Predicted: 2.05×10^{-10}

Image not found

beta-Caryophyllene

Measured: 2.00×10^{-10}

Predicted: 1.99×10^{-10}